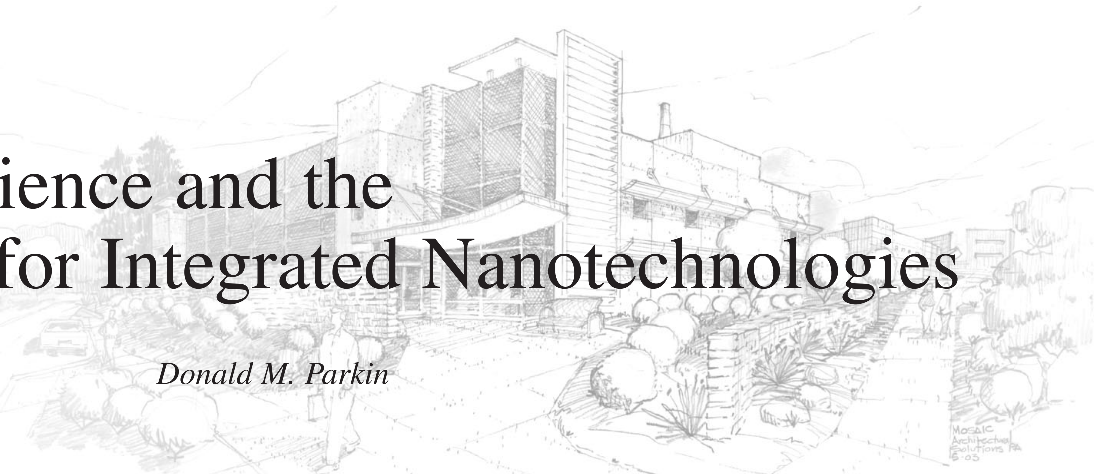


Nanoscience and the Center for Integrated Nanotechnologies

Donald M. Parkin

Science and technology are on the verge of a revolution, fueled by what Dr. John Marburger, President Bush's science advisor, calls "the atom-by-atom understanding of functional matter." The revolution goes by the name of "nanotechnology," and it offers a dazzling range of possibilities for observing the functioning of living systems, modifying the functional properties of materials, and designing atomic-scale structures with entirely new properties.

In broad terms, nanotechnology researchers seek to understand and exploit systems of atoms and molecules that are partly governed by structure on length scales of 1 to 100 nanometers. For perspective, a row of 10 hydrogen atoms would span about 1 nanometer. At the nanometer scale, the boundaries between traditional scientific disciplines and realms of expertise begin to fade. Thus, the key to fulfilling the promise of nanotechnology is an integration of the traditionally separate science disciplines—physics, chemistry, materials science, and biology—coupled to a robust program in computation and engineering.

At Los Alamos, we believe that nanotechnology will be a critical component of our efforts to meet mission responsibilities in national security, threat reduction, energy, and fundamental science. It will enable improvements in chemical and nuclear sensing, high-performance military platforms, and nuclear defense systems and lead to the creation of biosensor systems that can detect emerging diseases or biothreats. Nanotechnology promises a similar revolution in medical diagnostics and therapeutics through the development of new drug formulations and delivery methods.

The National Nanotechnology Initiative was launched in 2000 as a coordinated government program to address national nanotechnology objectives. In response to that initiative, Los Alamos and Sandia National Laboratories jointly created the Center for Integrated Nanotechnologies (CINT). Formally a Nanoscale Science Research Center of the Department of Energy Office of Science, CINT is devoted to establishing the scientific principles that govern the design, performance, and integration of nanoscale materials. It is one of five such centers throughout the country.

CINT operates as a national user facility and provides the external user community—university faculty, students, other national laboratory scientists, and industrial researchers—with no-cost, open, and peer-reviewed access to the center's capabilities and expertise. Los Alamos operates two additional national user facilities, the National High Magnetic Field Laboratory and the neutron scattering facility at the Los Alamos Neutron Science Center. (See the article "The LANSCE National User Facility" on page 138.) Both facilities will provide critical capabilities to the CINT activity.

The science capabilities that CINT will nurture and develop derive from the combined capabilities at Los Alamos and Sandia. We have focused on five such capabilities, the first involving the intersection of microbiology with nanoscale materials, or what we call the "nano-bio-micro-interface." This is an especially challenging area of research.

One goal is to use nanoscale biomolecular and bio-inspired assemblies to create functional microscale or larger devices. An example might be a pathogen detection system, wherein an organic receptor (which would recognize and bind to the pathogen) couples directly to an inorganic sensor platform. Another far-reaching goal is to develop new materials whose structure, function, and assembly are inspired by natural systems. In either case, the central challenge of this capability is to gain control of the physical interface between the biomolecular and synthetic materials. We hope to develop biofunctional and biocompatible surfaces and understand how to assemble biomolecular components at interfaces. We also hope to develop new approaches to the study of biological systems, approaches that will be based on new nanoscale materials and material characterization tools.

Within the nanophotonics and nanoelectronics capability, we seek to understand and control fundamental electronic and photonic interactions in nanostructured materials. The properties of electrons in tiny bits of semiconductor material, for example, become significantly modified as the bits shrink in size to 10 nanometers or less. Appropriately termed "quantum dots," these nanoscale pieces of matter behave in some ways like bulk materials, and in others, like single atoms.

By gaining an understanding of their electronic properties, we have been able to turn quantum dots into a new type of optical-gain media, culminating in our demonstration of a color-selectable, quantum dot laser. (See the article “Nanocrystal Quantum Dots” on page 214.) In addition, we hope to develop nanostructures that are significantly more complex than existing materials, incorporating multiple constituents, finer length scales, and new three-dimensional architectures. Like the nano-bio-micro capability, the research will be strongly supported by instrument development.

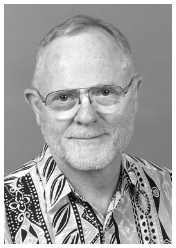
In the area of complex functional materials, we will explore new materials and their routes to synthesis, materials that promote complex and collective interactions between individual nanoscale components. The approach is to investigate self-assembly processes, relevant interfacial phenomena, approaches to hierarchical organization of materials, and integration strategies to access phenomena not available in individual components. Many of these activities are realized in Los Alamos work that is devoted to synthesizing field-effect transistors from molecular crystals. Here, the basic semiconductor can be self-assembled from molecules with specific functionality, and the major challenge is to control the interface between conventional electronic materials and the molecular crystal. This work is directed toward a new generation of electronic materials that are flexible and can cover large areas.

Increasing our understanding of the mechanisms underlying the mechanical behavior of nanoscale materials and structures is the direction of the nanomechanics capability. The scientific challenges in this area are to synthesize new materials with novel mechanical properties based on tailored nanostructures. We hope to understand how structuring at the nanometer length scale influences mechanical responses (such as energy dissipation), coupling, and nonlinearities.

Theory and simulation fit well with the experimentally focused capabilities previously described. State-of-the-art computational resources will help us address the complex, multiple length-scale problems. A key opportunity arises from the fact that oftentimes, nanostructured materials have responses that are dictated by structure length scales, which are readily accessible to computer modeling methods. Using simulations, we can explore the structure of biomolecular assemblies, nanostructured interfaces, and self-assembled nanoscale materials, as well as optical and electronic structures. For example, we want to model and simulate the mechanical properties of organic crystals in a polymer matrix, whose individual constituents have dimensions in the nanoscale. We are also performing calculations of the phosphorylation reactions catalyzed by kinase enzymes.

A New Center

To provide state-of-the-art equipment and a cooperative research environment, the CINT program is currently overseeing $76 million worth of construction that will culminate in a 96,000 square-foot Core Facility in Albuquerque, New Mexico, and a 34,000 square-foot Gateway Facility in Los Alamos, both to be in operation by 2006. Together with an existing Gateway at Sandia, these three facilities will provide space for researchers to synthesize and characterize nanostructured materials, theoretically model and simulate their performance, and integrate nanoscale materials into larger-scale systems. CINT will jump-start its user program in 2003 before the new facilities are complete. It will leverage existing resources at Los Alamos and Sandia and carefully build its user program in collaboration with the national and international science communities, so that by 2006 it will have both a fully operating user program and state-of-the-art facilities. The inherently multidisciplinary nature of these CINT building blocks will foster interdisciplinary research teams. It is from the integration of CINT capabilities with Laboratory and external scientist teams, new state-of-the-art facilities, and existing nanoscale science resources with grand challenge problems that we derive our name, the Center for Integrated Nanotechnologies.■



Donald Parkin graduated from the University of Utah with a Ph.D. in physics in 1970. After a four-year career at Brookhaven National Laboratory, he joined Los Alamos in 1974 and worked on radiation effects modeling. Don joined the management of the Center for Materials Science in 1984 where he was the Director from 1988 through 1999. He served as the MST Deputy Division Leader from 2000 through 2002. In 2002 he became the Associate Director of the Center for Integrated Nanotechnologies and the leader of MST-CINT. Don is the Program Manger for the DOE Division of Materials Sciences and Engineering. His activities in nanotechnology are focused on making CINT into a world leading nanoscience resource for the nation.